

2-amino-3-(4-chlorophenyl)sulfonylpropanoic acid
5445-04-5 | DTXSID30396827

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 54.8 L/kg

Global applicability domain: Inside

Local applicability domain index: 4.77e-01

Confidence level: 6.53e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Asulam</div> <div>Measured: 39.8</div> <div>Predicted: 38.8</div>	<div>Image not found</div> <div>Thidiazuron</div> <div>Measured: 110</div> <div>Predicted: 141</div>	<div>Image not found</div> <div>Phenazopyridine</div> <div>Measured: 209</div> <div>Predicted: 268</div>
<div>Image not found</div> <div>Aldoxycarb</div> <div>Measured: 2.63</div> <div>Predicted: 5.32</div>	<div>Image not found</div> <div>Cyanazine</div> <div>Measured: 191</div> <div>Predicted: 253</div>	